Methyl beta-alanate

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.13

Global applicability domain: Inside

Local applicability domain index: 5.39e-01

Confidence level: 7.94e-01

Nearest Neighbors from the Training Set

Image not found
N-(Hydroxyethyl)ethylenediamine
Measured: 2.88
Predicted: 3.29

Image not found
Piperazine
Measured: 3.89
Predicted: 2.44

Image not found
Morpholine
Measured: 2.82
Predicted: 1.87

Image not found
3-Pyridinamine
Measured: 2.09
Predicted: 3.04

Image not found
4-Aminopyridine
Measured: 4.57
Predicted: 3.04